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MODELING AND CHARACTERIZATION OF PHONON TRANSMISSION

RONGGUI YANG
REGENTS OF THE UNIVERSITY OF COLORADO THE

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Final Report

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14. ABSTRACT
The Air Force is increasingly relying on the benefits of novel multifunctional materials. These materials are being pushed to their thermal limits in progressively more demanding roles. Therefore, there is a strong need to develop modeling and characterization tools for better understanding of thermal transport in nanostructured functional materials. The objective of this project is to develop an integrated modeling and characterization tool to study phonon transmission and generation across engineered and strained interfaces. Such a tool will be critical in understanding the fundamentals of energy transport and in developing structure-property relations of functional nanostructures that could enable novel design of multi-functional nanostructures with superior thermal properties, such as super-thermal insulators, high efficiency thermoelectric materials, and super-thermal conductors. The accomplishment of this project include: 1). developed an atomic Green's function based-method for phonon transmission calculations, 2). developed a novel approach to measure phonon mean free path, and 3). studied the thermal transport in a few emerging materials such as hybrid organic-inorganic materials and two-dimensional materials such as transition metal dichalcogenides.

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Modeling and Characterization of Phonon Transmission and Generation across Engineered and Strained Interfaces for Developing Structure-Property Relations of Functional Nanostructures

(FA9550-11-1-0109)
Performance Period: June 15, 2011 – December 14, 2014

Ronggui Yang
Department of Mechanical Engineering, University of Colorado at Boulder

The Air Force is increasingly relying on the benefits of novel multifunctional materials. These materials are being pushed to their thermal limits in progressively more demanding roles. Therefore, there is a strong need to develop modeling and characterization tools for better understanding of thermal transport in nanostructured functional materials. **The objective of this project** is to develop an integrated modeling and characterization tool to study phonon transmission and generation across engineered and strained interfaces. Such a tool will be critical in understanding the fundamentals of energy transport and in developing structure-property relations of functional nanostructures that could enable novel design of multi-functional nanostructures with superior thermal properties, such as super-thermal insulators, high efficiency thermoelectric materials, and super-thermal conductors.

The Innovation and Accomplishments of this project include:

1). Developed modeling and simulation tools for thermal and thermoelectric transport processes across interfaces and in nanostructured materials. In particular, we have developed a novel approach to predict phonon transport properties across dissimilar interfaces. Our approach is based on non-equilibrium Green's function theory (NEGF) which provides a wavelength-dependent phonon transmission function. This approach has been integrated with the molecular dynamics simulations and the first-principles simulations to predict phonon transmission function across strained and engineered materials interfaces. The obtained wavelength-dependent phonon transmission function will be integrated into the Boltzmann transport model to study and design large-scale multidimensional systems with embedded nanostructures. The results were published in Journal of Physics: Condensed Matter (Vol. **24**, Art # 155302, 2012), Physical Review B (Vol. 86, Art #054305, 2012), and a recently accepted paper in Physical Review B (Xiaokun Gu, *et al*, Phonon transmission across $Mg_2Si/Mg_2Si_{1-x}Sn_x$ interface: a first-principles-based atomistic Green's function study, http://arxiv.org/abs/1501.04084, May 2015)

2). In an earlier work published in Nature Materials (Vol. 9, pp. 26-30, 2010), we developed a pump-and-probe characterization tool using table-top femtosecond extreme ultraviolet (EUV) laser to study nanoscale thermal transport. In the experiment, an array of nanowires made by electron-beam lithography is heated with an ultrafast laser pulse, and the heat flow from the nanowire array into a bulk substrate is monitored by diffracting ultrafast coherent EUV beams from the nanostructure. This allowed us to make the first observation of the ballistic heat flow regime at nanoscale interfaces and quantitatively measure the strength of the ballistic effect. During this project period, we have focused on the measurement of nanoscale heat transfer

surrounding even smaller heat sources (down to a linewidth of 25nm). We uncovered a new and surprising regime of nanoscale thermal transport that dominates when the separation between nanoscale heat sources is comparable with phonon mean free paths – a regime that has not been observed or predicted to date. We find that, very counterintuitively, nanoscale heat sources spaced closely together can cool more quickly than widely-spaced heat sources of the same size! This most recent discovery has been published in PNAS - Proceedings of the National Academy of Sciences of the United States of America (Vol. 112, pp.4846-4851, 2015). Such a discovery gives unprecedented method to characterize the differential thermal conductivity contributions of phonons with different MFPs and to benchmark predictions from first-principles density functional theory (DFT) calculations.

3). We have made significant progresses in the understanding of thermal transport in emerging materials. Working with our collaborators world-wide, we have studied thermal transport in many nanostructured materials, including hybrid organic-inorganic crystals, thin films fabricated using atomic layer deposition (ALD) and molecular layer deposition (MLD) techniques, and most recently the emerging two-dimensional materials including graphene, silicone, and transition metal dichalcogenides.

In the following, we highlight some of the afore-mentioned achievements:

Thrust #1. A first-principles-based atomistic Green's function study on phonon transmission across dissimilar materials.

In recent years, the atomistic Green's function (AGF) approach has been shown to be an efficient method to study frequency-dependent phonon transport across interfaces of dissimilar materials. The phonon transmission is highly dependent on the details of atomic configuration and interatomic interaction around the interface. AGF approach has been applied to study a wide range of interfaces, including sharp (smooth) interfaces, rough interfaces, interfaces with vacancy defects and alloyed interfaces. Often the empirical potentials are used in AGF calculations to describe the interatomic interactions. The interatomic force constants from the first-principles calculations have also been integrated with AGF method for studying interfaces of materials, especially when the empirical potentials are not readily available.

However, it would be quite challenging to extract the interatomic force constants of realistic material interfaces from the first-principles calculations. Comparing to the first-principles prediction of thermal conductivity of bulk crystals, the lattice near an interface of two dissimilar materials is likely to be distorted due to the lattice mismatch and the difference in the force field experienced by the atoms in the interfacial region. A large supercell would be required for the first-principles calculations to capture the essential characteristics of the lattice-mismatched interface, which leads to severe numerical challenges. The mass approximation (MA) that was employed to calculate the thermal conductivity of alloys has thus been used to extract interatomic force constants of the interfacial region from the first-principles. Under the MA, the differences in the lattice constants and the force fields between the two dissimilar materials are ignored and only the difference in atomic mass is taken into account. It was recently pointed out that the MA tends to overestimate the thermal conductivity due to the neglect of the local force-field difference. Other studies showed that the MA under-predicts the contribution of high-

frequency phonons, which leads to a lower thermal conductivity. It is unclear whether MA is a reasonable approximation when integrated with the AGF approach to calculate the phonon transmission across the interfaces of dissimilar materials where there exist the differences in both lattice constants and force fields.

In this work, we proposed an integrated first-principles-based AGF approach using higher-order force constant model (HOFCM) to compute phonon transmission across interfaces of dissimilar materials, with the details shown in ***Figure 1.***

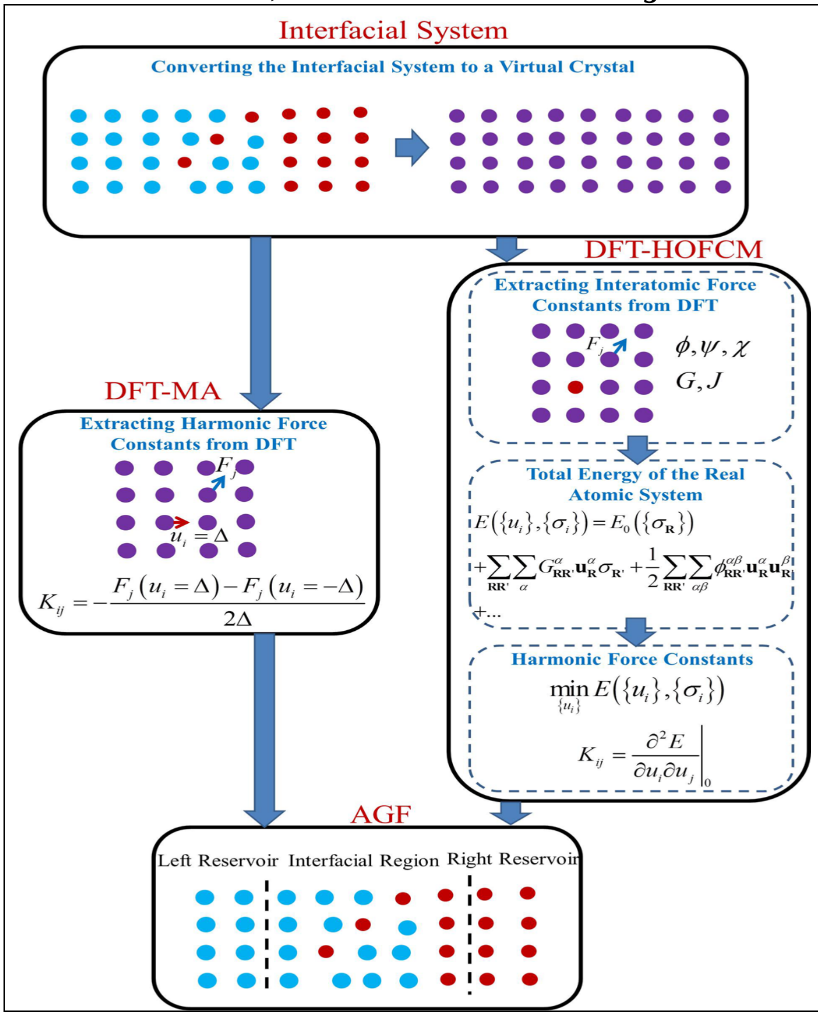

Figure 1. Numerical simulation procedure of the integrated DFT-AGF approaches: MA-AGF and HOFCM-AGF. In both approaches, an interfacial system is first converted to an effective virtual crystal. In MA, the harmonic force constants are computed from DFT calculations of the virtual crystal, and then directly used as the inputs for AGF calculations. In HOFCM, the interatomic force constants with respect to both the atom displacements and atom species are extracted from DFT calculations. Then a force-field using these interatomic force constants are constructed, which is used to determine the equilibrium configuration of the interfacial system and the corresponding harmonic force constants that are used in AGF calculations.

By considering the lattice distortion and the species-dependent local force field, the accuracy of the interatomic force constants extracted is improved compared with that from the MA, while the required computational resources are significantly less severe than directly extracting force constants from the standard first-principles calculations. As an example, we conducted the detailed studies of frequency-dependent phonon transmission across $Mg_2Si/Mg_2Si_{1-x}Sn_x$ interface, as shown in ***Figure 2***, which is promising thermoelectric material system for intermediate temperature range energy conversion applications. We systematically study how the lattice mismatch-induced local force field influences phonon transmission across the interfaces between dissimilar materials, which are inevitably ignored in the MA. This study could provide guidance for designing nanostructured materials with tunable thermal conductivity.

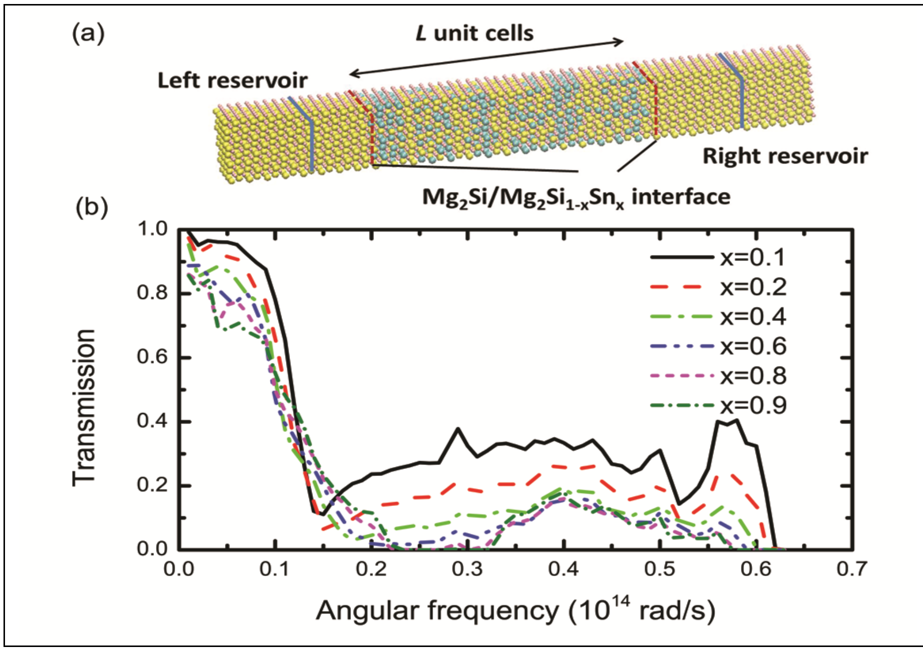

Figure 2. (a) The schematic of the simulation system of $Mg_2Si/Mg_2Si_{1-x}Sn_x/Mg_2Si$ structure. (b). Phonon transmission across the $Mg_2Si/Mg_2Si_{1-x}Sn_x/Mg_2Si$ structure as a function of phonon frequency for different Sn compositions (x). The length of the alloy layers is fixed at 10 unit cells.

Thrust #2. phonon mean free paths measurement technique using extreme ultraviolet laser-enabled pump-and-probe method.

The Fourier's law of heat conduction considers heat transport as a diffusive process where energy flow is driven by a temperature gradient. However, at length scales smaller than the mean free path for the energy carriers, heat flow becomes ballistic - driven by direct point-to-point transport of energy quanta. Although past experiments have seen ballistic effects in layered thin films or nanowires, non-Fourier heat dissipation from a nanoscale hot spot to the surrounding had not been experimentally observed and was a subject of some uncertainty although it has significant relevance in heat dissipation of electronic transistors In an earlier work published in Nature Materials (Vol. 9, pp. 26-30, 2010), we developed a pump-and-probe characterization tool using table-top femtosecond extreme ultraviolet (EUV) laser to study nanoscale thermal transport. In the experiment, an array of nanowires made by electron-beam lithography is heated with an ultrafast laser pulse, and the heat flow from the nanowire array into a bulk substrate is monitored by diffracting ultrafast coherent EUV beams from the nanostructure. This allowed us to make the first observation of the ballistic heat flow regime at nanoscale interfaces and quantitatively measure the strength of the ballistic effect. Such an experimental discovery of ballistic phonon transport a surrounding nanoscale heat source along with the recent advances on computational prediction of phonon mean free path distributions using the first-principles-based density functional theory have inspired a few research groups in exploring the measurements of phonon mean free path distributions in crystalline materials using ultrafast optical wavelength laser-based pump and probe method [Regner, K. T. et al. Nat. Commun. **4,** 1640 (2013). Minnich, A. J. et al. Phys. Rev. Lett. **107,** 095901 (2011). Johnson, J. A. et al. Phys. Rev. Lett. **110,** 025901 (2013).].

However, the basic proof-of-principle using optical wavelength lasers has limited to the contribution of long-wavelength (> 1 μm) MFP phonons in silicon. During this project period,

we have focused on the measurement of nanoscale heat transfer surrounding even smaller heat sources (down to a linewidth of 25nm) using the table-top femtosecond EUV laser-enabled pump-and-probe method. We uncovered a new and surprising regime of nanoscale thermal transport that dominates when the separation between nanoscale heat sources is comparable with phonon mean free paths – a regime that has not been observed or predicted to date. We find that, very counterintuitively, nanoscale heat sources spaced closely together can cool more quickly than widely-spaced heat sources of the same size! This most recent discovery has been published in PNAS - Proceedings of the National Academy of Sciences of the United States of America (Vol. 112, pp.4846-4851, 2015). Such an experimental demonstration of the regime map of nanoscale heat transport gives unprecedented method to characterize the differential thermal conductivity contributions of phonons with different MFPs and to benchmark predictions from first-principles density functional theory (DFT) calculations. As shown in ***Figure 3***, the experimental data of the size-dependent effective thermal resistivity (conductivity) for sapphire and silicon substrates were used to extract the phonon mean free path distributions by using the suppression function which identifies the contributions of phonon modes with each mean free path range. To extract the phonon MFP distributions, the experimental data were fit with the weights $k(\Lambda_i)$ assigned to multiple bins of phonon modes which give their average relative contribution to the differential thermal conductivity (purple shading). ***Figure 3*** shows that the experimental data on cumulative thermal conductivity and phonon mean free path distributions agrees well with DFT calculation, which offers the first experimental benchmark for first-principle calculations.

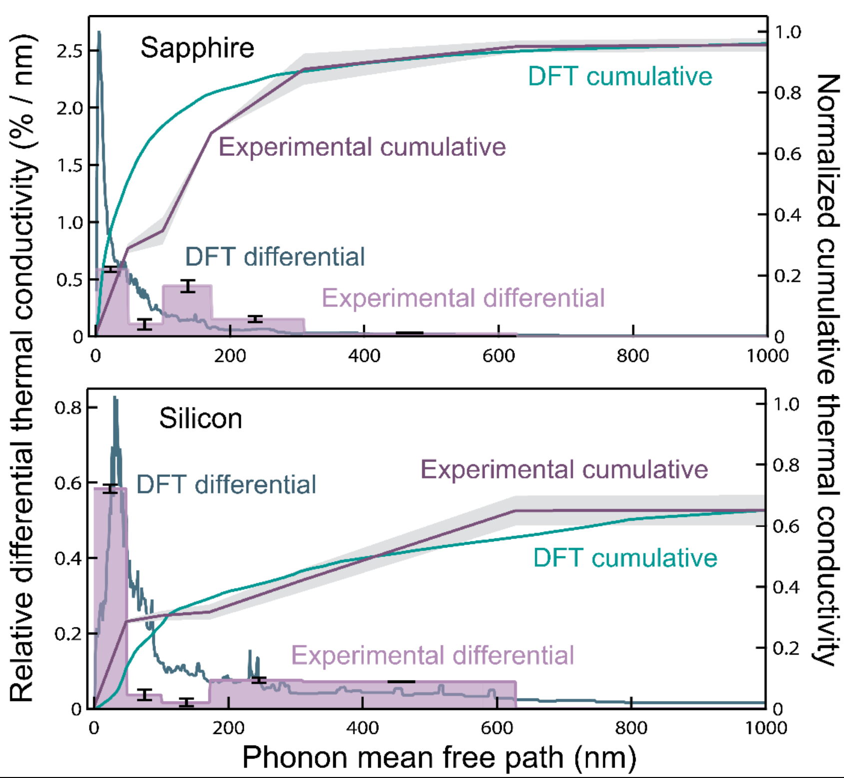

Figure 3. *The experimental data on effective thermal resistivity (conductivity) from nanoscale heat source was used to extract the cumulative thermal conductivity and differential thermal conductivity due to the contributions of phonon with different mean free paths. The phonon mean free path distributions measured agree well with DFT calculation.*

Thrust #3. Modeling and measurement of thermal transport in emerging materials.

Working with our collaborators world-wide, we have studied thermal transport in many nanostructured materials, including hybrid organic-inorganic crystals, thin films fabricated using atomic layer deposition (ALD) and molecular layer deposition (MLD) techniques, and most recently the emerging two-dimensional materials including graphene, silicone, and transition metal dichalcogenides.

Two-dimensional transition metal dichalcogenides (TMDCs) are finding promising electronic and optical applications due to their unique properties. In this work, we systematically study the phonon transport and thermal conductivity of eight semiconducting single-layer TMDCs, MX_2 (M=Mo, W, Zr and Hf, X=S and Se), as shown in ***Figure 4***, by using the first-principles-driven phonon Boltzmann transport equation approach. The validity of the single-mode relaxation time approximation to predict the thermal conductivity of TMDCs is assessed by comparing the results with the iterative solution of the phonon Boltzmann transport equation. A very high thermal conductivity value of 142 W/mK was found in single-layer WS_2. The large atomic weight difference between W and S leads to a very large phonon bandgap which in turn forbids the scattering between acoustic and optical phonon modes and thus resulting in very long phonon relaxation time, as shown in ***Figure 5***.

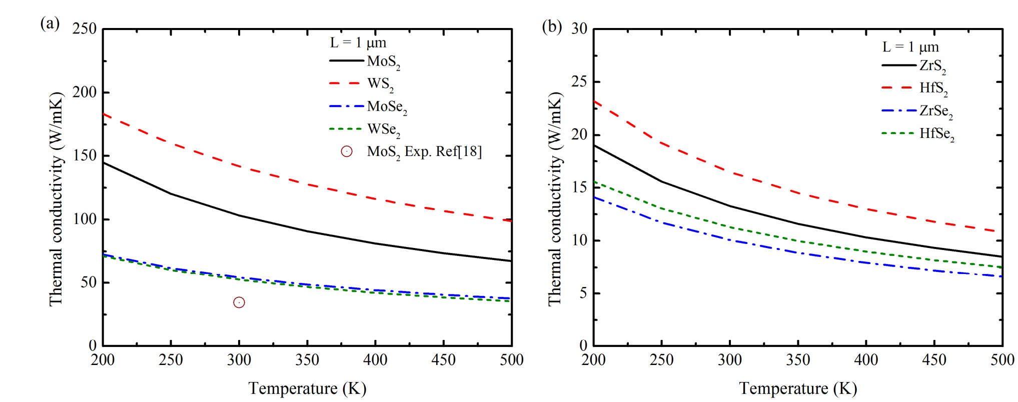

Figure 4. *The thermal conductivity of (a) 2H and (b) 1T TMDC monolayers as a function of temperature.*

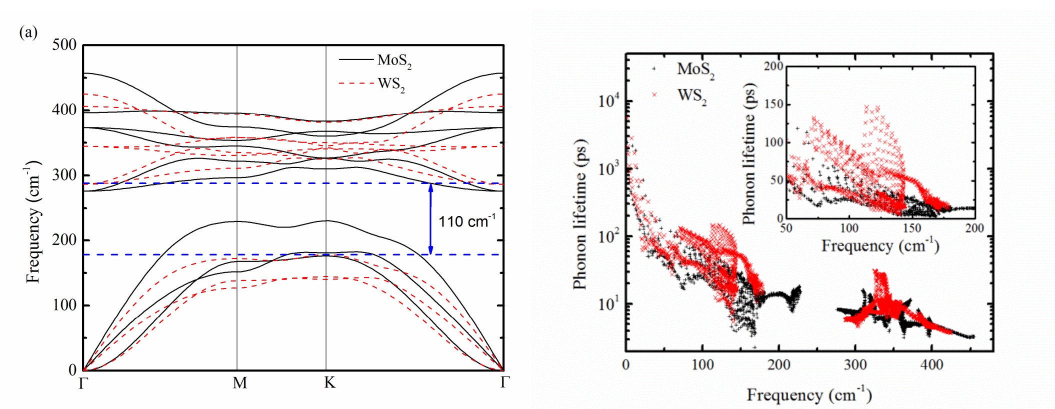

Figure 5. *Phonon dispersion (a) and lifetime (b) of MoS_2 and WS_2 calculated from the first-principles simulations.*

Journal Papers Published or Accepted

Thrust #1:

1. Xiaokun Gu, Xiaobo Li and Ronggui Yang, Phonon Transmission across $Mg_2Si/Mg_2Si_xGe_{1-x}$ Interfaces: an Integrated First-Principles and Atomic Green's Function Approach, Physical Review B, Accepted, http://arxiv.org/abs/1501.04084, May 2015.
2. Xiaobo Li, and Ronggui Yang, Effect of Lattice Mismatch on Phonon Transmission and Interface Thermal Conductance across Dissimilar Material Interfaces, Physical Review B, Vol. 86, Art #054305 (13 pages), 2012.
3. Xiaobo Li, and Ronggui Yang, Size-Dependent Phonon Transmission across Interfaces of Dissimilar Materials, Journal of Physics: Condensed Matter, Vol. 24, Art # 155302 (12 pages), 2012.
4. Tuhin Shuvra Basu, Ronggui Yang, Suraj Joottu Thiagarajan, Siddhartha Ghosh, Stanislaw Gierlotka, and Mallar Ray, Remarkable Thermal Conductivity Reduction in Metal-Semiconductor Nanocomposites, Applied Physics Letters, Vol. 103, Art #083115 (5 pages), 2013.
5. Jun Liu, Shenghong Ju, Yifu Ding, and Ronggui Yang, Size Effect on the Thermal Conductivity of Ultrathin Polymers, Applied Physics Letters, Art # (4 pages), 2014.

Thrust #2:

6. Kathleen M. Hoogeboom-Pot, Jorge N. Hernandez-Charpak, Travers D. Frazer, Xiaokun Gu, Erik H. Anderson, Weilun Chao, Roger W. Falcone, Ronggui Yang, Margaret M. Murnane, Henry C. Kapteyn and Damiano Nardi, A New Regime of Nanoscale Thermal Transport: Collective Diffusion Counteracts Dissipation Inefficiency, PNAS - Proceedings of the National Academy of Sciences of the United States of America, Vol. 112, pp.4846-4851, 2015
7. Jun Liu, Byunghoon Yoon, Eli Kuhlmann, Miao Tian, Xiaokun Gu, Steven M. George, Yung-Cheng Lee, and Ronggui Yang, Ultra-Low Thermal Conductivity of Atomic/Molecular Layer Deposited (ALD/MLD) Hybrid Organic-Inorganic Thin Films, Nano Letters, Vol. 13, pp. 5594-5599, 2013.
8. Jun Zhou, Nianbei Li, and Ronggui Yang, An Electrohydrodynamic Model for Non-equilibrium Electron and Phonon Transport in Metal Films after Ultra-short Pulse Laser Heating, European Physics Journal B, Accepted, http://arxiv.org/abs/1408.0426.
9. J. Ordonez-Miranda, and Ronggui Yang, Sebastian Volz and J.J. Alvarado-Gil, Steady-State and Modulated Temperature Profiles in Layered Systems Predicted by the Phonon Boltzmann Transport Equation, Journal of Applied Physics, Accepted, http://arxiv.org/abs/1501.03174

Thrust #3:

10. Yujie Wei, Jiangtao Wu, Hanqing Yin, Xinghua Shi, Ronggui Yang, Mildred S. Dresselhaus, The Nature of Strength Enhancement and Weakening by Pentagon-Heptagon Defects in Graphene, Nature Materials, Vol. 11, pp. 759–763, 2012.

11. Yujie Wei, Baoling Wang, Jiangtao Wu, Ronggui Yang, and Martin L. Dunn, Bending Rigidity and Gaussian Bending Stiffness of Single-Layered Graphene, Nano Letters, Vol. 13, pp. 26-30, 2013.
12. Jiangtao Wu, Baolin Wang, Yujie Wei, Ronggui Yang, Mildred Dresselhaus, Mechanics and Mechanically Tunable Bandgap in Single-Layer Hexagonal Boron-Nitride, Materials Research Letters, Vol. 1, n4, pp. 200-206, 2013.
13. Baolin Wang, Jiangtao Wu, Xiaokun Gu, Hanqing Yin, Yujie Wei, Ronggui Yang, and Mildred Dresselhaus, Stable planar single-layer hexagonal silicene under tensile strain and its anomalous Poisson’s ratio, Applied Physics Letters, Applied Physics Letters, Vol. 104, Art #081902 (5 pages), 2014
14. Xiaokun Gu, and Ronggui Yang, Phonon Transport in Single-Layer Transition Metal Dichalcogenides: a First-Principles Study, Applied Physics Letters, Vol. 105, Art #131903 (5 pages), 2014.
15. Xiaokun Gu, and Ronggui Yang, First-Principles Prediction of Phononic Thermal Conductivity of Silicene: A Comparison with Graphene, Journal of Applied Physics, Vol. 117, Art #025102, 2015.
16. Chunlei Wan, Xiaokun Gu, Feng Dang, Tomohiro Itoh, Yifeng Wang, Hitoshi Sasaki, Mami. Kondou, Kenji Koga, Kazuhisa Yabuki, G. Jeffrey Snyder, Ronggui Yang, and Kunihito Koumoto, " Flexible N-type thermoelectric materials by organic intercalation of layered transition metal dichalcogenide TiS_2”, Nature Materials, published online: http://dx.doi.org/10.1038/nmat4251

Thrust #4: Coupled Electron and Phonon (Thermoelectric) Transport, Effective Medium Theory

17. Jun Zhou, Ronggui Yang, Gang Chen and Mildred S. Dresselhaus, Optimal Bandwidth for High Efficiency Thermoelectrics, Physical Review Letters, Vol. 107, Art # 226601 (5 pages), 2011.
18. Jun Zhou, and Ronggui Yang, Quantum and Classical Thermoelectric Transport in Quantum Dot Nanocomposites, Journal of Applied Physics, Vol. **110**, Art # 084317 (12 pages), 2011.
19. Jun Zhou, and Ronggui Yang, Ballistic Thermoelectric Transport in Double-Bend Nanowires, Applied Physics Letters, Vol. 98, Art# 173107 (3 pages), 2011.
20. Yuanyuan Wang, Jun Liu, Jun Zhou, and Ronggui Yang, Thermoelectric Transport across Polymer-Semiconductor-Polymer Nanoscale Junctions, Journal of Physical Chemistry C, Vol. 117, pp. 24716-24725, 2013.
21. Jose Ordonez-Miranda, Ronggui Yang, and J.J. Alvarado-Gil, A New Constitutive Equation for Nano-to-Macro- Scale Heat Conduction Based on Boltzmann Transport Equation, Journal of Applied Physics, Vol. 109, Art # 084319 (8 pages), April 2011.
22. Jose Ordonez-Miranda, Ronggui Yang, and J.J. Alvarado-Gil, The Effect of the Electron-Phonon Coupling on the Effective Thermal Conductivity of Metal-Nonmetal Multilayers, Journal of Applied Physics, Vol. 109, Art #094310 (7 pages), May 2011.
23. David Makhija, Georg Pingen, Ronggui Yang, and Kurt Maute, Topology Optimization of Multi-component flows by Multi-relaxation Time Lattice Boltzmann Method, Computers and Fluids, Vol. 67, pp. 104–114, 2012.
24. Ordonez-Miranda, J. J. Alvarado-Gil and Ronggui Yang, Effective Thermal Conductivity of Particulate Composite at Non-Dilute Limit, Journal of Applied Physics, Vol. **114**, Art #064306, 2013.

Honors and Awards Received by Professor Ronggui Yang during the Project Period 2011-2014:
2014 ITS Young Investigator Award, International Thermoelectric Society (ITS)
2013-2017 S.P. Chip and Lori Johnson Faculty Fellow of Engineering, CU-Boulder.
2013 Outstanding Research Award, Department of Mechanical Engineering, CU-Boulder
2013 JSPS Invitation Fellow (Short Term), Japan Society for the Promotion of Science.
2012 Provost's Faculty Achievement Award, Office of the Provost, CU-Boulder.
2011 Steve Woodward Outstanding Faculty Award, Department of Mechanical Engineering, CU-Boulder

Honors and Awards Received by Professor Yang's Advisees Working on this Project:
Mr. Xiaokun Gu, Tees Family Endowed Fellowship, from College of Engineering and Applied Physics, University of Colorado, Boulder.
Jun Liu, Best Dissertation Award from College of Engineering and Applied Physics in 2013-2014 (One out of 80 PhD Graduates), University of Colorado, Boulder.
Jun Liu, the Third Place Prize of NSF student poster competition in ASME/IMECE 2013 in San Diego, CA.
Jun Liu, NSF Travel Award for attending ASME/IMECE 2013 in San Diego, CA.
Xiaokun Gu, NSF Travel Award for attending ASME/IMECE 2013 in San Diego, CA.
Jose Ordonez, IPPA Junior Prize 2013, the International Photoacoustic and Photothermal Association (IPPA).
Jun Liu, Best Presentation of The DayAward for Graduate Engineering Annual Research & Recruitment Symposium (GEAR^{2}S), Universityof Colorado at Boulder, 2013.
Jose Ordonez, National Prize for Best Dissertation in Natural Sciences, Mexico, 2012.
Jun Liu, the First Place Prize of NSF CBET/CMMI student poster competition in ASME/IMECE 2012.
Xiaokun Gu, the Second Place Prize of NSF CBET/CMMI student poster competition in ASME/IMECE 2012.
Xiaokun Gu, NSF Travel Award for attending ASME/IMECE 2012 in Houston, TX.
Jun Liu, NSF Travel Award for attending ASME/IMECE 2012 in Houston, TX.
Jun Liu, March 2012, "Most Excited Molecules" for his presentation at 12th GEAR^{2}S Conference, Mechanical Engineering, CU-Boulder.

Professional Service Activities by Professor Yang During the Project Period:

a). Technical Committees
07/2015 – 06/2017, Chair, K-9 Technical Committee on Nanoscale Thermal Transport, ASME Heat Transfer Division.
07/2014 – 06/2016, Chair, Nanoengineering for Energy and Sustainability (NEES) Steering Committee, ASME Nanoengineering Council.
2013 - present, Committee Member, ASME K-7 & AICHE Joint Technical Committee on Thermophysical Properties, ASME Heat Transfer Division & AICHE.
2012 – 06/2015, Founding Vice Chair, K-9 Technical Committee on Nanoscale Thermal Transport, ASME Heat Transfer Division.

2012 – 06/2014, Vice Chair, Nanoengineering for Energy and Sustainability (NEES) Steering Committee Member, ASME Nanoengineering Council.
2009 - 2013, Committee Member, K-8 Technical Committee on Fundamentals and Theory of Heat Transfer, ASME Heat Transfer Division.
2009 – 2012, Committee Member, Nanoengineering for Energy and Sustainability Steering Committee (NEES), ASME Nanoengineering Council.

b). Journal Editor
2014- present, Associate Editor, ASME Journal of Electronic Packaging.
2014- present, Editorial Board Member, Scientific Reports, published by Nature Publishing Group.

c). Conference Recently Organized/Co-Organized
Topic Co-Organizer, Thermal Properties of Nanostructured Materials, the
19th ASME/AICHE/NIST Symposium on Thermophysical Properties, Boulder, CO, June 21-26, 2015.
Chair, Best Poster Award Committee, the 2nd International Conference on Phononics and Thermal Energy Science, Tongji University, Shanghai, China, May 26-31, 2014.
Session Chair, the 2nd International Conference on Phononics and Thermal Energy Science, Tongji University, Shanghai, China, May 26-31, 2014.
Track Co-Chair, Track #9 Thermal Metrology at Micro/Nanoscales, The 4th ASME Micro/Nanoscale Heat & Mass Transfer International Conference (MNHMT-13), The University of Hongkong, Hongkong, China, December 11 – 14, 2013
Topic Co-Organizers, Nanoengineering for Energy and Sustainability, ASME International Mechanical Engineering Conference and Exhibitions (ASME IMECE), San Diego, CA, Nov. 2013.
Topic Organizer, Nanoscale Thermal Transport (15 Technical Sessions), ASME IMECE, San Diego, CA, Nov. 2013.
Topic Co-Organizers, Nanoengineering for Energy and Sustainability, (Session Chair or Co-Chair of 6 technical sessions in this topic under 10-4, managed the review for 28 abstracts), ASME IMECE, Houston, TX, Nov 11-15, 2012.
Topic Organizer with two Co-Organizers, Fundamentals of Nanoscale Heat Transport, (Session Chair or Co-Chair of 7 technical sessions in this topic under 7-3, managed the review for 40 abstracts and 25 full papers), ASME IMECE, Houston, TX, Nov 11-15, 2012.
Topic Organizer with two Co-Organizers, Fundamentals of Phase-Change Heat Transport, (Session Chair or Co-Chair of 7 technical sessions in this topic under 7-3, managed the review for 40 abstracts and 20 full papers), ASME IMECE, Houston, TX, Nov 11-15, 2012.
Topic Co-Organizer (managed the review for 42 abstracts, chaired 2 out of 7 technical sessions organized), Thermal Properties of Nanostructured Materials, the 18th ASME/AICHE/NIST Symposium on Thermophysical Properties, Boulder, CO, June 24-29, 2012.
Track Co-Organizer, Track #4 Nanoengineering for Energy and Sustainability (6 technical sessions), ASME IMECE, Denver, CO, November 2011.
Topic Co-Organizer, Fundamentals of Nanoscale Heat Transport (12 technical sessions), ASME IMECE, Denver, CO, November 2011.
Topic Organizer, Fundamentals and Applications of Phase-Change Heat Transport (7 technical sessions), ASME IMECE, Denver, CO, November 2011.

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University of Colorado

Grant/Contract Title
The full title of the funded effort.

Modeling and Characterization of Phonon Transmission and Generation across Engineered and Strained Interfaces for Developing Structure-Property Relations of Functional Nanostructures

Grant/Contract Number
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Ronggui Yang

Program Manager
The AFOSR Program Manager currently assigned to the award

John Luginsland

Reporting Period Start Date

06/15/2011

Reporting Period End Date

12/14/2014

Abstract

The Air Force is increasingly relying on the benefits of novel multifunctional materials. These materials are being pushed to their thermal limits in progressively more demanding roles. Therefore, there is a strong need to develop modeling and characterization tools for better understanding of thermal transport in nanostructured functional materials. The objective of this project is to develop an integrated modeling and characterization tool to study phonon transmission and generation across engineered and strained interfaces. Such a tool will be critical in understanding the fundamentals of energy transport and in developing structure-property relations of functional nanostructures that could enable novel design of multi-functional nanostructures with superior thermal properties, such as super-thermal insulators, high efficiency thermoelectric materials, and super-thermal conductors.

The Innovation and Accomplishments of this project include:

1). Developed modeling and simulation tools for thermal and thermoelectric transport processes across interfaces and in nanostructured materials. In particular, we have developed a novel approach to predict phonon transport properties across dissimilar interfaces. Our approach is based on non-equilibrium Green's function theory (NEGF) which provides a wavelength-dependent phonon transmission function. This approach has been integrated with the molecular dynamics simulations and the first-principles simulations to predict phonon transmission function across strained and engineered materials interfaces. The obtained wavelength-dependent phonon transmission function will be integrated into the Boltzmann transport model to study and design large-scale multidimensional systems with embedded nanostructures. The results were published in Journal of Physics: Condensed Matter (Vol. 24, Art # 155302, 2012), Physical Review B (Vol. 86, Art #054305, 2012), and a recently accepted paper in Physical Review B (Xiaokun Gu, et al, Phonon transmission across Mg2Si/Mg2Si1-xSnx interface: a first-principles-based atomistic Green's function study, http://arxiv.org/abs/1501.04084, May 2015)
2). In an earlier work published in Nature Materials (Vol. 9, pp. 26-30, 2010), we developed a pump-and-probe characterization tool using table-top femtosecond extreme ultraviolet (EUV) laser to study nanoscale thermal transport. In the experiment, an array of nanowires made by electron-beam lithography is heated with an ultrafast laser pulse, and the heat flow from the nanowire array into a bulk substrate is monitored by diffracting ultrafast coherent EUV beams from the nanostructure. This allowed us to make the first observation of the ballistic heat flow regime at nanoscale interfaces and quantitatively measure the strength of the ballistic effect. During this project period, we have focused on the measurement of nanoscale heat transfer surrounding even smaller heat sources (down to a linewidth of 25nm). We uncovered a new and surprising regime of nanoscale thermal transport that dominates when the separation between nanoscale heat sources is comparable with phonon mean free paths – a regime that has not been observed or predicted to date. We find that, very counterintuitively, nanoscale heat sources spaced closely together can cool more quickly than widely-spaced heat sources of the same size! This most recent discovery has been published in PNAS - Proceedings of the National Academy of Sciences of the United States of America (Vol. 112, pp.4846-4851, 2015). Such a discovery gives unprecedented method to characterize the differential thermal conductivity contributions of phonons with different MFPs and to benchmark predictions from first-principles density functional theory (DFT) calculations.
3). We have made significant progresses in the understanding of thermal transport in emerging materials. Working with our collaborators world-wide, we have studied thermal transport in many nanostructured materials, including hybrid organic-inorganic crystals, thin films fabricated using atomic layer deposition (ALD) and molecular layer deposition (MLD) techniques, and most recently the emerging two-dimensional materials including graphene, silicone, and transition metal dichalcogenides.

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Archival Publications (published) during reporting period:

1. Xiaokun Gu, Xiaobo Li and Ronggui Yang, Phonon Transmission across Mg2Si/Mg2SixGe1-x Interfaces: an Integrated

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2. Xiaobo Li, and Ronggui Yang, Effect of Lattice Mismatch on Phonon Transmission and Interface Thermal Conductance across Dissimilar Material Interfaces, Physical Review B, Vol. 86, Art #054305 (13 pages), 2012.
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Changes in research objectives (if any):

N/A

Change in AFOSR Program Manager, if any:

N/A

Extensions granted or milestones slipped, if any:

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AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

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Appendix Documents

2. Thank You

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